# Density Gradient calibration for 2D quantum confinement : Tri-Gate SOI transistor application

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*Abstract*— This article presents a Density-Gradient (DG) calibration for 2D quantum confinement on Tri-Gate Silicon on insulator cross section for which the top gate interface is <100>-oriented and the lateral gate interfaces are <110>-oriented. To calibrate the DG model, we use self-consistent Poisson-Schrödinger calculations and fit the capacitance vs gate voltage (C-V) curves. We first calibrate DG model for one-dimensional quantum confinement (1D) on planar devices cross section for both crystal orientations. Then, we check the validity of the parameters obtained for the two-dimensional (2D) quantum confinement on tri-gate architecture cross-section. The DG model allows a good description of the C-V curves in the case of 2D quantum confinement and the parameters are still valid when we reduce the Tri-Gate cross section up to 4 nm by side.

Keywords—Density-Gradient; Tri-Gate; Calibration; Schrödinger-Poisson; crystal orientations

## I. INTRODUCTION

As Metal-Oxide-Semiconductor field-effect transistors (MOSFETs) reach nanometer dimensions, exploration of alternative devices is required. Three-dimensional (3D) architectures are one of the most promising candidates for future technological nodes, mainly due to their particular improvement of the electrostatic control compared to conventional planar devices [1]. The literature provides a wide range of devices based on 3D architecture: stacked [2], twin [3] or single  $\Omega$ -FET nanowires [4].

Technology Computer-Aided Design (TCAD) [5] simulation provides essential tools to quantify the relevance of these new architectures by supporting technological developments and process optimization. It is widely recognized that quantum effects are significant in Tri-Gate devices and one of the main TCAD challenges is therefore to reproduce correctly these effects. For this, we used the well-known Density Gradient (DG) approach developed by Ancona [6,7]. The classical strategy [8] is to calibrate all parameters in different crystal orientations by fitting both capacitance and carrier density. The reference code used here for calibration is the Poisson -Schrödinger solver provided in the TB\_Sim code [9].

The main purpose of the present paper is to detail the calibration of the DG model with a 2D Schrödinger-Poisson (PS) by fitting the DG  $\gamma$  parameter in the different crystal orientations for Tri-Gate transistor application. For this







Fig. 2. Capacitance vs Gate voltage for planar p- and n-type transistors with <100> substrate orientation (a) and <110> substrate orientation (b). Comparison between TCAD simulation (solid line) and 1D numerical Schrödinger-Poisson simulation (dashed). TBOX=20nm, H=20nm.



Fig. 3. Electron density for planar n-type transistors a) 100-oriented and b) 110-oriented, and hole density for planar p-type transistors c) 100-oriented and d) 110-oriented. Comparison between TCAD simulation (solid line) and 1D numerical Schrödinger-Poisson simulation (dashed). TBOX=20nm, H=20nm. VG=0.5V.

purpose, part II of the paper presents the Density-Gradient and the Schrödinger-Poisson models. In part III, the DG calibration in planar devices for 100 and 110 orientations for both n and p-type transistors is shown. In part IV, the parameters obtained in part III using 2D simulations are validated and we discuss on the limitation of this quantum confinement correction for the 3D MOSFET architecture.

#### II. MODELS USED

#### A. The Density-Gradient model

In TCAD software, the electronic transport is described within the Drift-Diffusion approach which corresponds to semi-classical approximation based on Boltzmann transport equation. One of the main problem is to include the effect of quantum confinement without solving Poisson-Schrödinger; for this we used the well-known Density-Gradient (DG) model [6,7]. The DG model is an approximation of quantum confinement effects coupled with transport equations. This approach is computationally efficient to take into account the quantum confinement, especially for 3D-TCAD simulation. The drift-diffusion equation is written as follows for electrons (eq. 1) and holes (eq. 2):

$$\frac{\partial n}{\partial t} = \frac{\nabla \cdot J_n}{q} = \nabla \cdot (-n\mu_n \nabla \Psi_n + D_n \nabla n) \tag{1}$$

$$\frac{\partial p}{\partial t} = \frac{\nabla \cdot J_p}{q} = \nabla \cdot (p\mu_p \nabla \Psi_p + D_p \nabla p)$$
(2)

where *n* and *p* are respectively the density of electrons and holes,  $\mu_n$  and  $\mu_p$  are their mobilities,  $J_n$  and  $J_p$  are their current densities, and  $\Psi_n$  and  $\Psi_p$  are their electric potentials. The electric potential is the sum of the classical electric potential  $\Psi$  and of the correction term through the quantum electric potential  $\Psi_{OM}$  :

$$\Psi_{n,p} = \Psi + \Psi_{QM} \tag{3}$$

For electron:

$$\Psi_{QM} = -\frac{\gamma_n \hbar^2}{6.m_n} \cdot \frac{\nabla^2 \sqrt{n}}{\sqrt{n}}$$
(4)

For hole:

$$\Psi_{QM} = -\frac{\gamma_p \hbar^2}{6.m_p} \cdot \frac{\nabla^2 \sqrt{p}}{\sqrt{p}}$$
(5)

where  $m_n$  and  $m_p$  are the density of state effective masses for electron and hole, respectively, and  $\gamma_n$  and  $\gamma_p$  are the keys parameters to calibrate the DG on PS simulations. Through the TCAD software, it is possible to fit the  $\gamma$  parameters for different orientation with auto orientation option (detailed on part III).

#### B. The Poisson-Schrödinger model

The Schrödinger-Poisson self-consistent calculations were performed with the TB Sim code [9]. Electrons and holes are described within the effective mass and the 6 bands k.p approximations, respectively. The Hamiltonians are discretized on a finite difference mesh with a step of 0.2 nm, which is small enough to ensure convergence of the charge density and of the potential. To check this, a few calculations were performed with a mesh step of 0.1 nm. An infinite potential barrier is considered at the Si/SiO<sub>2</sub> interface. This allows a better comparison with DG simulations, where the penetration into the oxide is not considered in this case. In the effective mass approximation, parabolic dispersion allows using Fermi-Dirac integrals to integrate the 2D (planar) and 1D (tri-gate) densities of states. For planar devices in the 6 bands k.p approximation, a polar sampling of the 2D Brillouin zone is used together with a spline interpolation [10]. For tri-gate devices, the 1D Brillouin zone is sampled with a regular mesh.

#### III. ONE-DIMENSIONAL CALIBRATION

In the first place, we calibrate DG parameters for 1D quantum confinement on a planar devices section. The setup of simulation is schematically reproduced on Fig. 1 a), the 1D stack is composed of : a metal gate at the top, 0.82 nm of Equivalent Oxide Thickness (EOT=0.82 nm), 20 nm of silicon layer (H=20 nm) and 20 nm of Buried Oxide ( $T_{BOX}$ =20 nm). We have simulated the capacitance vs gate voltage which represents the derivative of the total electron or hole density into the silicon film for each polarization in different (100) and (110) crystal orientations.

	nMOS		pMOS	
Orientation	100	110	100	110
γ	4.3	6.0	7.9	2.3
Tab. 1. $\gamma$ parameters for nMOS and pMOS for both (100) and (110).				



Fig. 4. Capacitance vs Gate voltage for p- and n-type Tri-Gate transistors. Comparison between TCAD simulation (solid line) and 2D numerical Schrödinger-Poisson simulation (dashed). TBOX=100nm, W=H=15nm.

To calibrate the  $\gamma$  parameter of the DG model, we first adjust the flat band voltage between the TCAD simulation and the PS reference. After this, we calibrate the  $\gamma$  parameter to find the minimum error on C-V curve. We obtain four different  $\gamma$  (cf. Table 1) for electron and hole for different crystal orientations. As detailed in Fig. 2.a and Fig. 2.b, we show the good agreement between PS and DG model on C-V curves.

To further investigate the quantum correction, figure 3 represents the electron density versus the position along the



Fig. 5. Electron density for n-type Tri-Gate transistors along a) vertical cut and b) horizontal cut. Comparison between TCAD simulation (solid line) and 2D numerical Schrödinger-Poisson simulation (dashed). TBOX=100nm, W=H=15nm. VG=0.5V



Fig. 6. Hole density for p-type Tri-Gate transistors along a) vertical cut and b) horizontal cut. Comparison between TCAD simulation (solid line) and 2D numerical Schrödinger-Poisson simulation (dashed). TBOX=100nm,W=H=15nm. VG=-0.5V

confinement direction for a specific polarization. The DG electron densities match with a good agreement with PS results, but it is not the case for hole densities. This mismatch is due to the use of 6 bands **k.p** approximation in PS simulations, which describes better the valence bands and shows the limitation of the DG model to capture correctly the valence band complexity. The hole density does not fit perfectly whereas the capacitance is well reproduced; in fact the capacitance represents the total charge into the silicon film whatever its distribution. Thus the error on the electron density on the peak and centroid near the interface is compensated by its spreading.

### IV. TWO-DIMENSIONAL VALIDATION

In the next place, we checked if the calibrated DG parameters can reproduce the PS results for two-dimensional problem. Tri-Gate section described Fig. 1 b) has been used for these comparisons. The crystal is <100>-oriented in the vertical direction and <110>-oriented in the horizontal direction. Figure 4 shows the C-V characteristics for Tri-Gate section with H=W=15 nm and we obtain a good agreement for pMOS and nMOS cases.

In accordance with the previous simulation on 1D structure (Fig. 3.b for electron and Fig 3.d for hole), the electron (Fig. 5.b) and hole (Fig. 6.b) density is very close to PS simulation in horizontal cut. In vertical cut, the discrepancy of the electron and hole density (Fig. 5.a for electron and 6.a for hole) compared to 1D case (Fig. 3.a for electron and Fig 3.c



Fig. 7. Capacitance vs gate voltage for various tri-gate dimensions W=H= 15, 10, 8, 6, 5 & 4 nm. Comparison between TCAD simulation (solid line) and 2D numerical Schrödinger-Poisson simulation (dashed). for pMOS and nMOS channels.

for hole) comes from the non-exact determination of the work function, especially with the impact of 2D potential distribution into BOX. However, this variation has negligible impact on the C-V curve.

The figure 7 shows capacitance versus the gate voltage curves for different silicon thickness and width. As expected, we obtain a good agreement between DG model with the corresponding  $\gamma$  parameter and PS simulation. In Fig. 8, the threshold voltages, defined at the maximum of the C-V derivative [11], are shown for different tri-gate dimensions. These results show that the pMOS calibration is less accurate than the nMOS case. In fact, this point highlights one of the limits of DG model that considers a unique effective mass for hole and do not take into account the valence band complexity. Moreover, this approach is also limited for Tri-Gate architecture upper than W=H=4 nm where effective masses strongly increase due to extreme confinement and the deformation of band diagram (as explained in [12]). Even if



Fig. 8. Threshold voltage for various tri-gate dimensions W=H=15, 10, 8, 6, 5 & 4 nm. Comparison between TCAD simulation (solid line) and 2D numerical Schrödinger-Poisson simulation (dashed). The threshold voltage is defined as the gate voltage at the maximum of the capacitance derivative.

DG does not reproduce correctly the hole density, these results show that DG model well describes the quantum behavior on C-V curve.

# V. CONCLUSION

In this work, we presented the Density-Gradient calibration for 2D quantum confinement on a Tri-Gate Silicon on insulator section where the channel crystal is <100>-oriented in the vertical direction and <110>-oriented in the horizontal direction. We used self-consistent Poisson-Schrödinger calculations as reference, to calibrate the DG model with the C-V curves. We first calibrated DG model for 1D quantum confinement on planar devices section for both orientations, and then, we checked the validity of the obtained parameters for 2D quantum confinement on Tri-Gate cross section. The DG is not accurate enough to describe the charge repartition, but it allows a good description of the C-V curves for 2D quantum confinement. Moreover parameters are still valid up to 4nm by side Tri-Gate cross section. This calibration is essential to evaluate and benchmark the performance of 3D architectures.

#### ACKNOWLEDGMENT

This work is partially founded by the IBM-STMicroelectronics-CEA/LETI-MINATEC Development Alliance and ANR QUASANOVA project.

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